

Bayesian calibration of simulation models using experimental data

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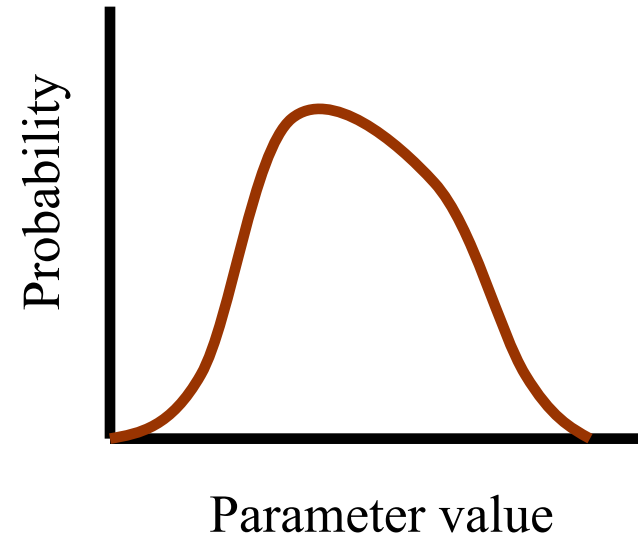
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Overview

- Bayesian calibration
 - ▶ more than parameter estimation
 - ▶ uncertainty quantification (UQ) is central issue
 - ▶ each new experiment used to improve knowledge of models
- Physics simulations codes
 - ▶ need to be understood on basis of experimental data
- Analysis process
 - ▶ employ hierarchy of experiments, from basic to fully integrated
 - ▶ goal is to learn as much possible from all experiments
- Example of analysis process: material model evolution
- Framework for Bayesian updating of sequence of expts.

Bayesian uncertainty analysis

- Uncertainties in parameters are characterized by probability density functions (pdf)
- Probability interpreted as quantitative measure of “degree of belief”
- Rules of classical probability theory apply
- Bayes law provides way to update knowledge about models as summarized in terms of uncertainty

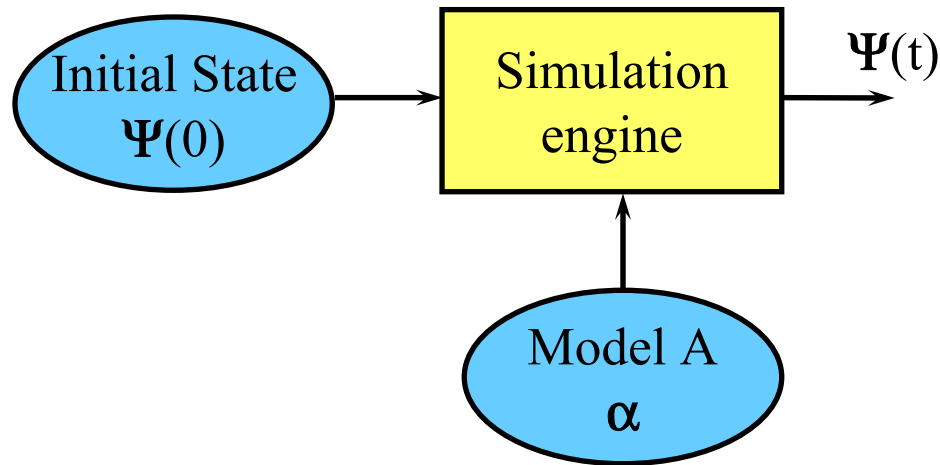


Bayesian calibration

Estimation of model parameters **and their uncertainties**

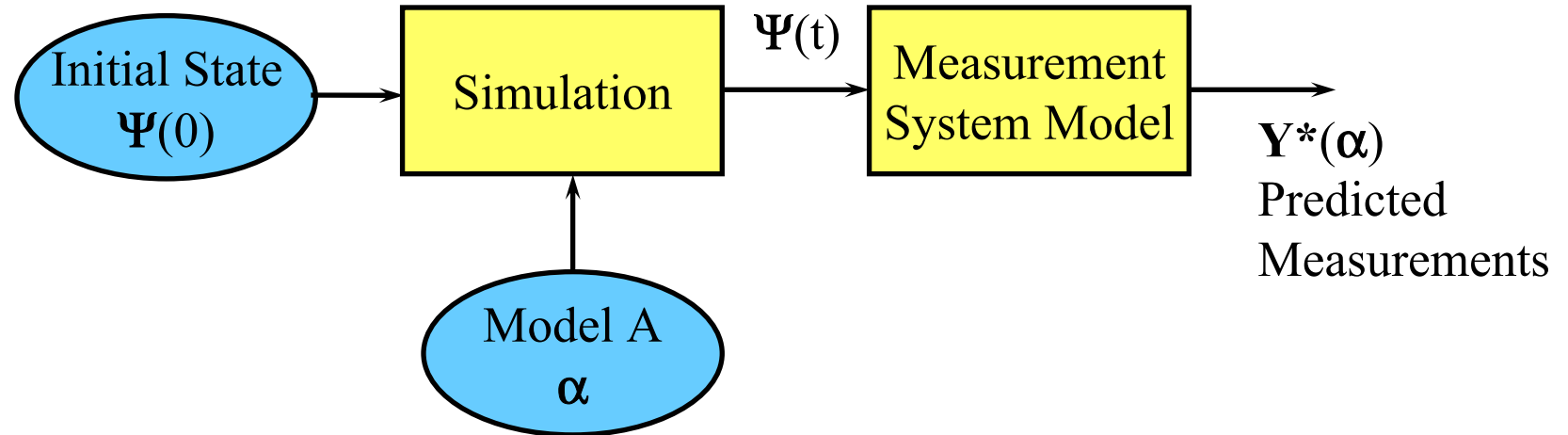
- Bayesian foundation
 - ▶ focus is as much on uncertainties in parameters as on their best value
 - ▶ use of prior knowledge, e.g., previous experiments
 - ▶ model checking;
does model agree with experimental evidence?

Schematic view of simulation code



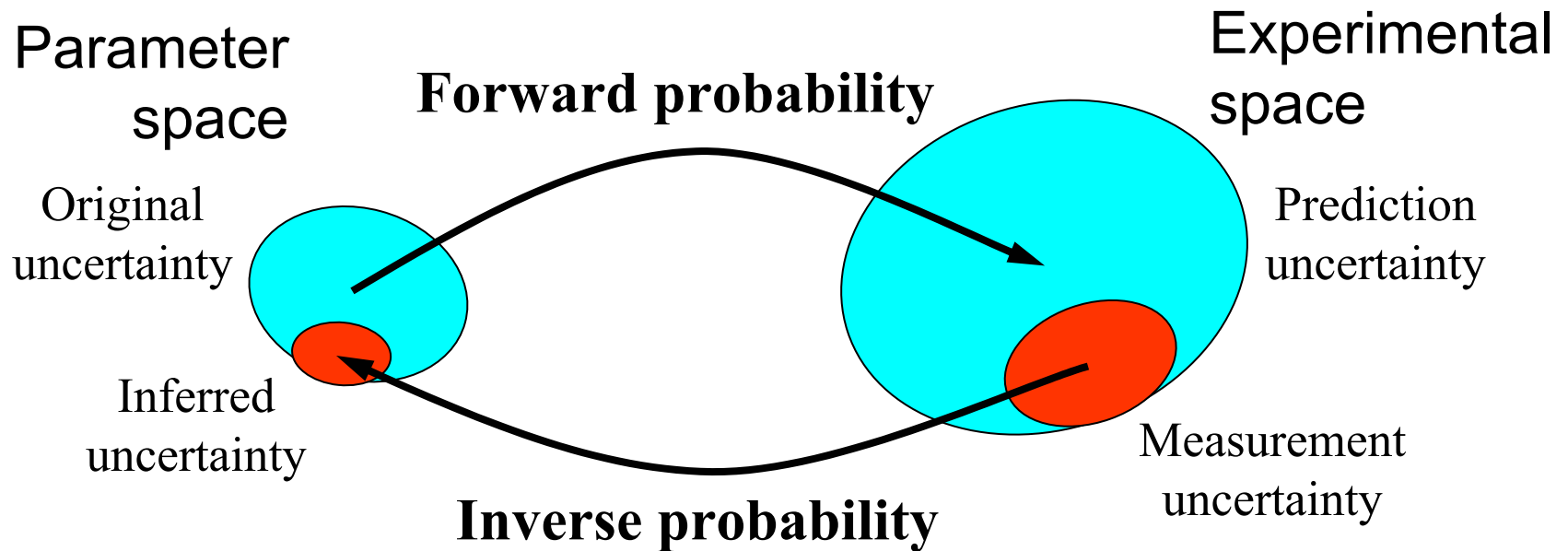
- Simulation code predicts state of time-evolving system
 $\Psi(t)$ = time-dependent state of system
- Requires as input
 - ▶ $\Psi(0)$ = initial state of system
 - ▶ description of physics behavior of each system component;
e.g., physics model A with parameter vector α (e.g., constitutive relations)
- Simulation engine solves the dynamical equations (PDEs)

Simulation code predicts measurements



- Simulation code predicts state of time-evolving system
 $\Psi(t)$ = time-dependent state of system
- Model of measurement system yields predicted measurements

Forward and inverse probability



- Model inference
 - ▶ if uncertainties in measurements are smaller than prediction uncertainties that arise from parameter uncertainties, one may be able to use measurements to reduce uncertainties in parameters
 - ▶ requires that prediction uncertainties are dominated by uncertainties in parameters and not by those in experimental set up
 - ▶ **good experimental technique** important for **Bayesian calibration**

Bayesian calibration for simulation codes

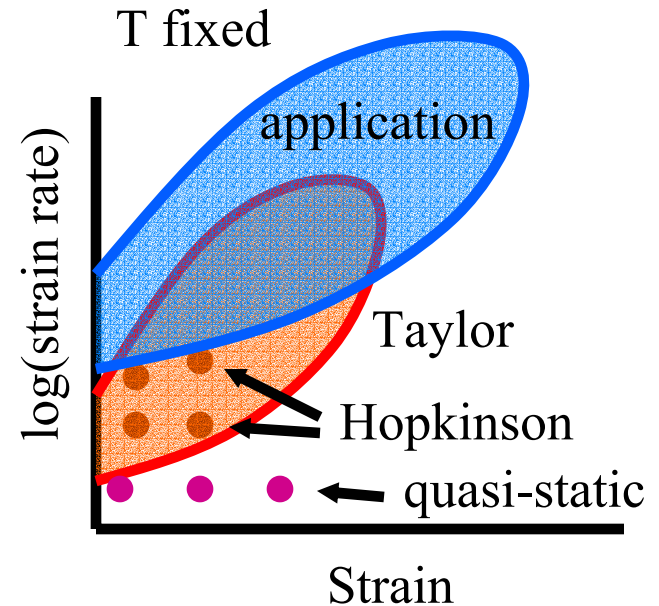
- Goal is to develop an uncertainty model for the simulation code by comparison to experimental measurements
 - ▶ determine and quantify sources of uncertainty
 - ▶ uncover potential inconsistencies of submodels with expts.
 - ▶ possibly introduce additional submodels, as required
- Recursive process
 - ▶ aim is to develop submodels that are consistent with all experiments (within uncertainties)
 - ▶ a hierarchy of experiments helps substantiate submodels over wide range of physical conditions
 - ▶ each experiment potentially advances our understanding

Motivating example

- Problem statement
 - ▶ design containment vessel using high-strength steel, HSLA 100
 - ▶ predict depth of vessel-wall penetration for specified shrapnel fragments at specified impact velocity
 - ▶ estimate uncertainty in this prediction to estimate safety factor
- Approach
 - ▶ determine what experiments are needed to characterize stress-strain relationship for plastic flow of metal
 - ▶ follow the uncertainty through the analysis of expt. data
 - ▶ variables to consider: temperature, strain rate, variability in material composition, processing, behavior

Hierarchy of experiments - plasticity

- Basic characterization experiments - measure stress-strain relationship at specific strain and strain rate
 - ▶ quasi-static – low strain rates
 - ▶ Hopkinson bar – medium strain rates
- Partially integrated expts. - Taylor test
 - ▶ covers range of strain rates
 - ▶ extends range of physical conditions
- Full integrated expts.
 - ▶ mimic application as much as possible
 - ▶ **projectile impacting plate**
 - ▶ may involve extrapolation of operating range; so introduces additional uncertainty
 - ▶ integrated expts. can help reduce model uncertainties

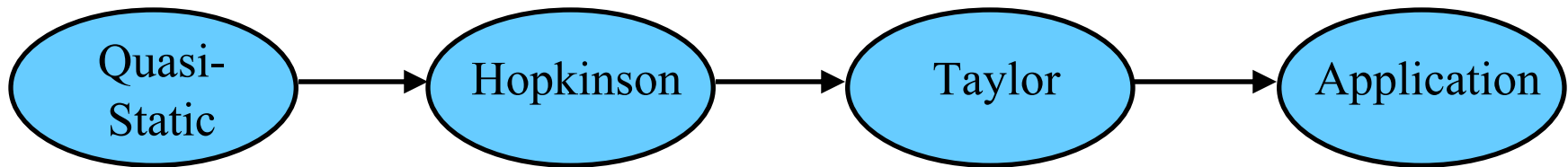


Analysis of hierarchy of experiments

**Basic
experiments**



**Fully integrated
application**

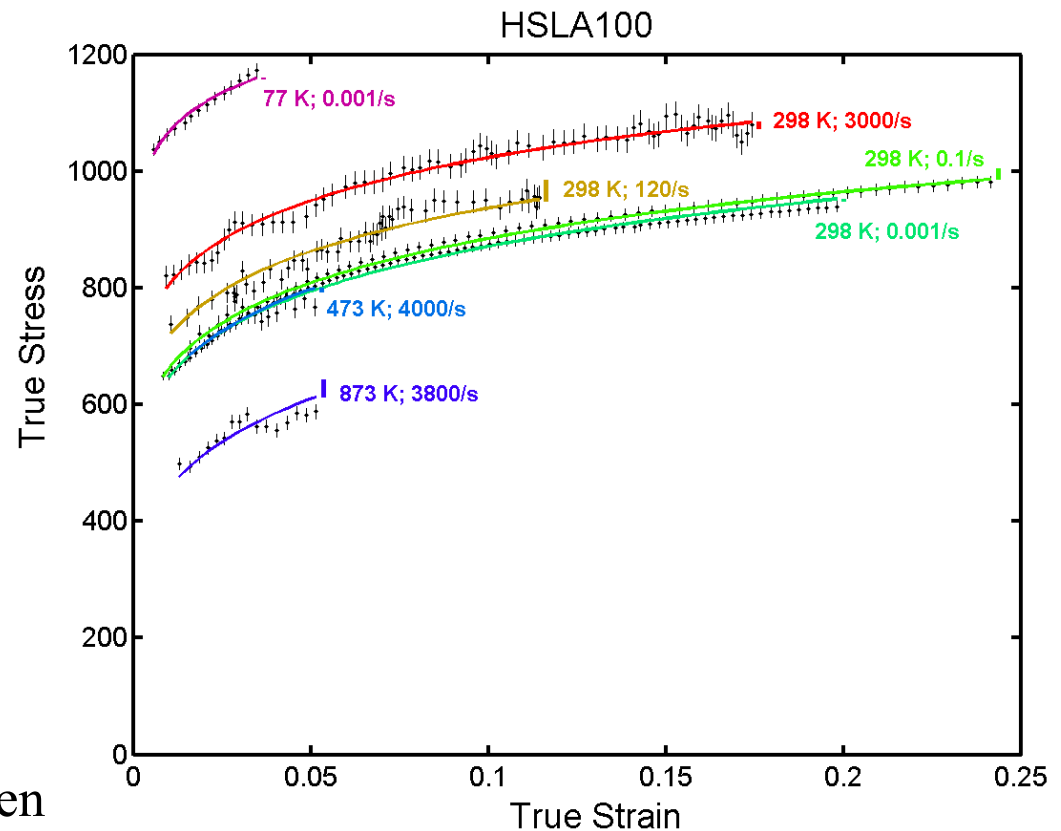


- Series of experiments to determine plastic behavior of a metal
- Information flow shown for analysis sequence
- Bayesian calibration –
 - ▶ analysis of each experiment updates model parameters and their uncertainties, consistent with previous experiments
 - ▶ information about models accumulates throughout process

Stress-strain relation for plastic deformation

Analysis of quasi-static and Hopkinson bar measurements†

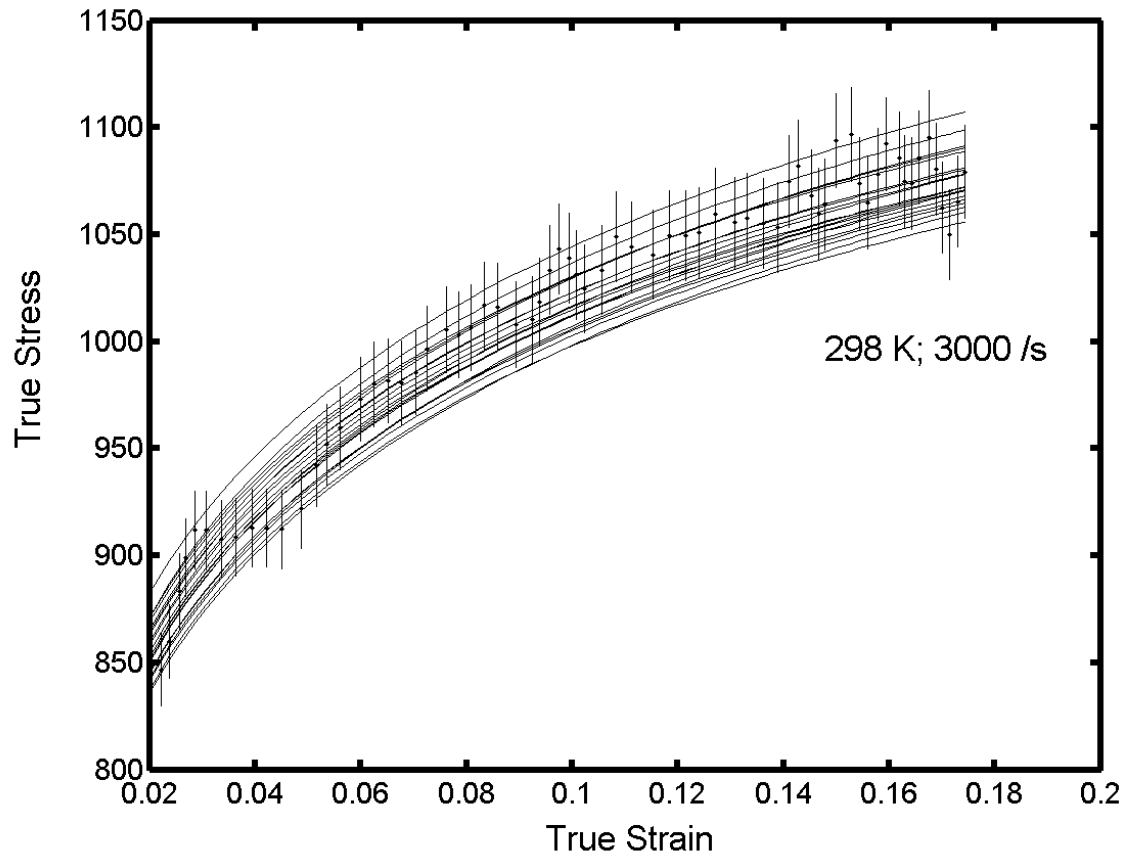
- Zerilli-Armstrong model for rate- and temperature-dependent plasticity
 - Parameters determined from Hopkinson bar measurements and quasi-static tests
 - Full uncertainty analysis – including systematic effects of offset of each data set (6 + 7 parms)
- $$\sigma = \alpha_1 + \alpha_5 \varepsilon_p^{\alpha_6} + \alpha_2 \exp \left[\left(-\alpha_3 + \alpha_4 \log \frac{\partial \varepsilon_p}{\partial t} \right) T \right]$$



†data supplied by Shuh-Rong Chen

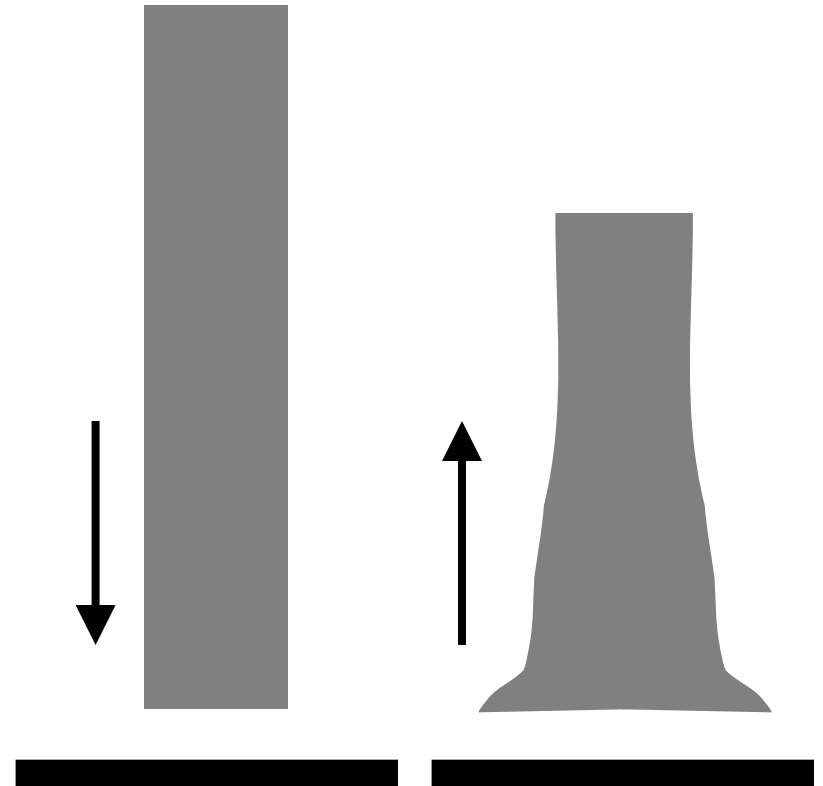
Monte Carlo sampling

- Use Monte Carlo to draw random samples from uncertainty distribution for Zerilli-Armstrong parameters



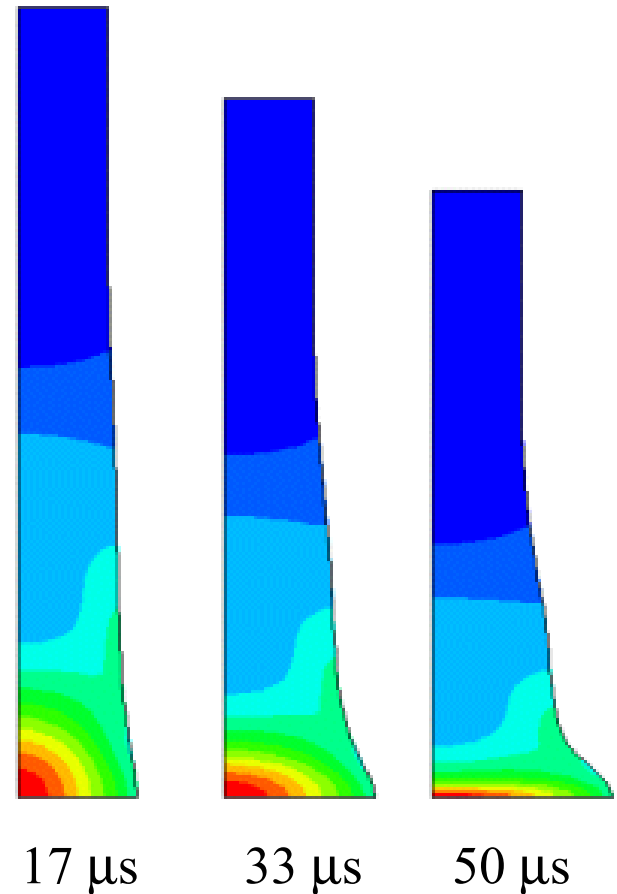
Taylor impact test

- Propel cylinder into rigid plate
- Measure profile of deformed cylinder
- Deformation depends on
 - cylinder dimensions
 - impact velocity
 - plastic flow behavior of material at high strain rate
- Useful for
 - determining parameters in material-flow model
 - validating simulation code (including material model)

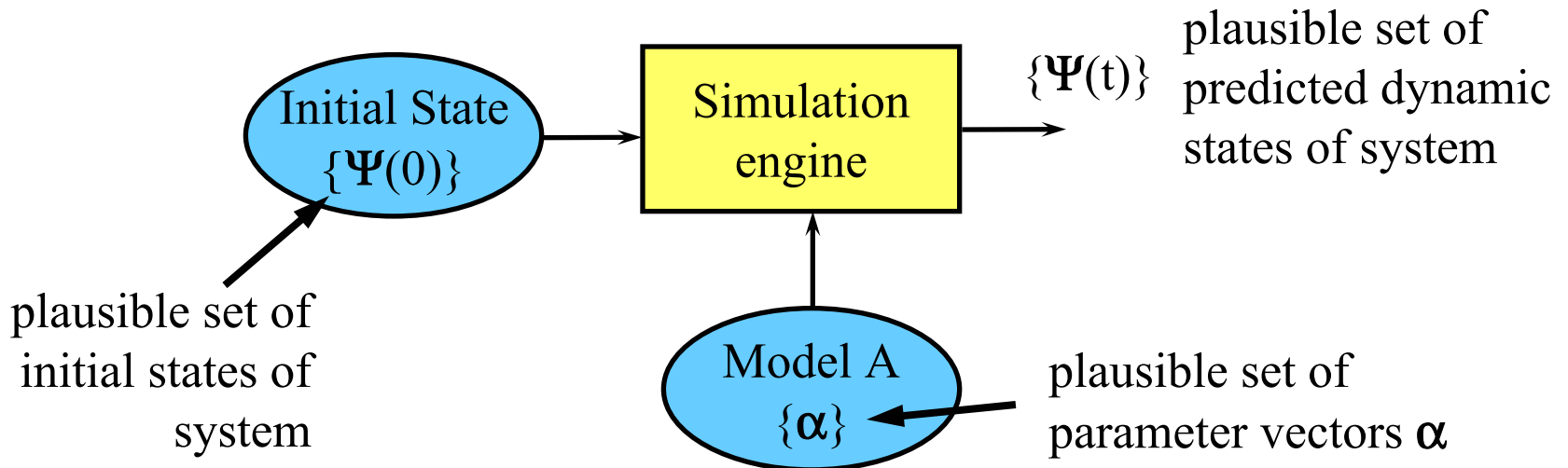


Taylor test simulations

- Simulate Taylor impact test
 - ▶ Abaqus, commercial FEM code
 - ▶ Johnson-Cook model for rate-dependent strength and plasticity
 - ▶ ignore anisotropy, fracture effects
 - ▶ cylinder: high-strength steel
15-mm dia, 38-mm long
 - ▶ impact velocity = 350 m/s
- Effective total strain reaches 250%



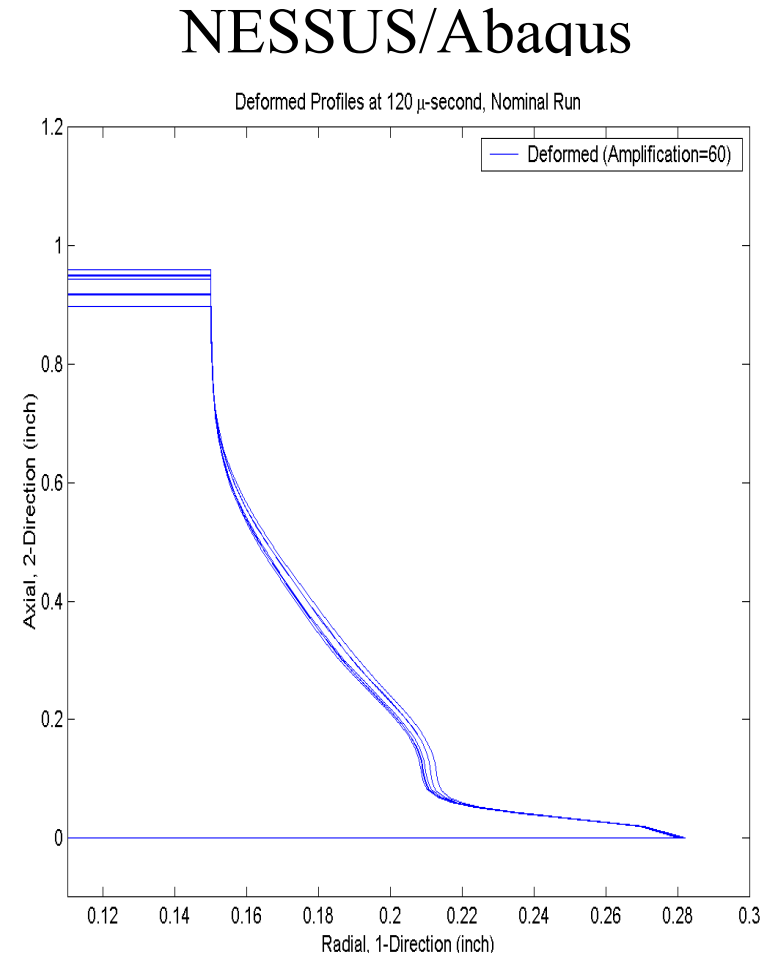
Plausible simulation predictions (forward)



- Generate plausible predictions for known uncertainties in parameters and initial conditions
- Monte Carlo method
 - ▶ run simulation code for each random draw from pdf for α , $p(\alpha|.)$, and initial state, $p(\Psi(0)|.)$
 - ▶ simulation outputs represent plausible set of predictions, $\{\Psi(t)\}$

Monte Carlo example - Taylor test

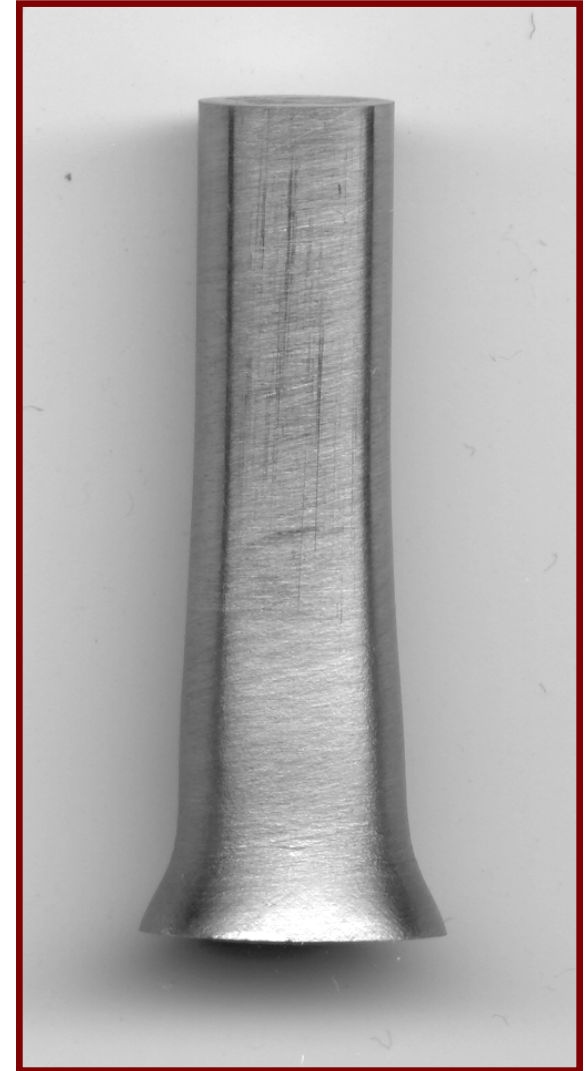
- Use MC technique to propagate uncertainties through deterministic simulation code
 - ▶ Draw value for each of four parameters from its assumed Gaussian pdf
 - ▶ Run Abaqus code for each set of parameters
- Figure shows range of variation in predicted cylinder shape



High-strength steel HSLA 100
246 m/s impact velocity

Taylor test experiment

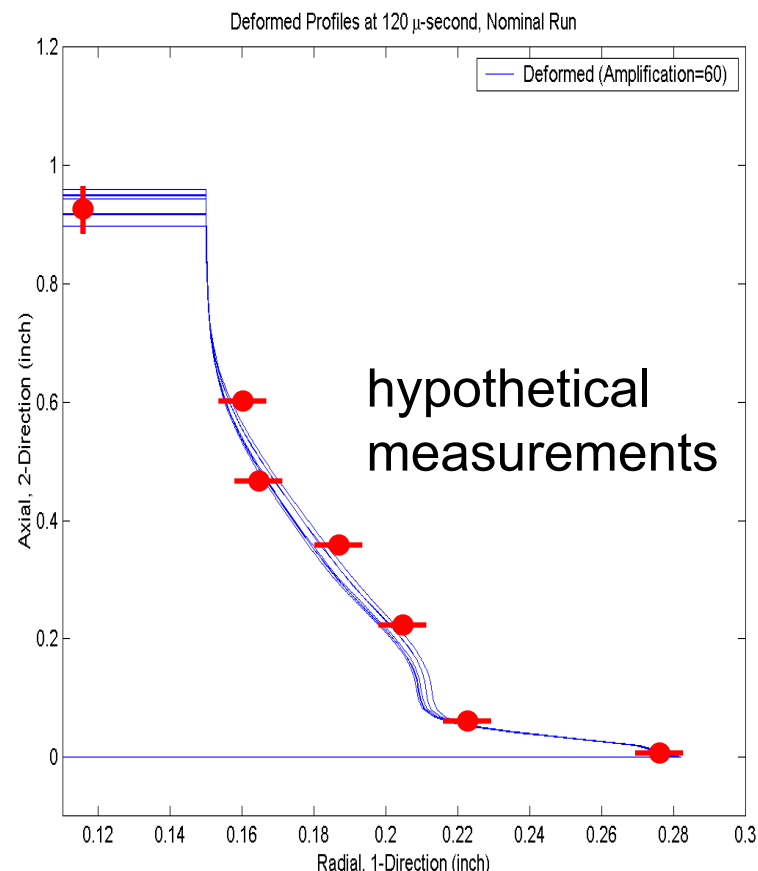
- Taylor impact test specimen
 - ▶ high-strength steel HSLA 100
 - ▶ impact velocity = 245.7 m/s
 - ▶ dimensions, final/initial
 - length 31.84 mm / 38 mm
 - diameter 12.00 mm / 7.59 mm



Comparison with experiment

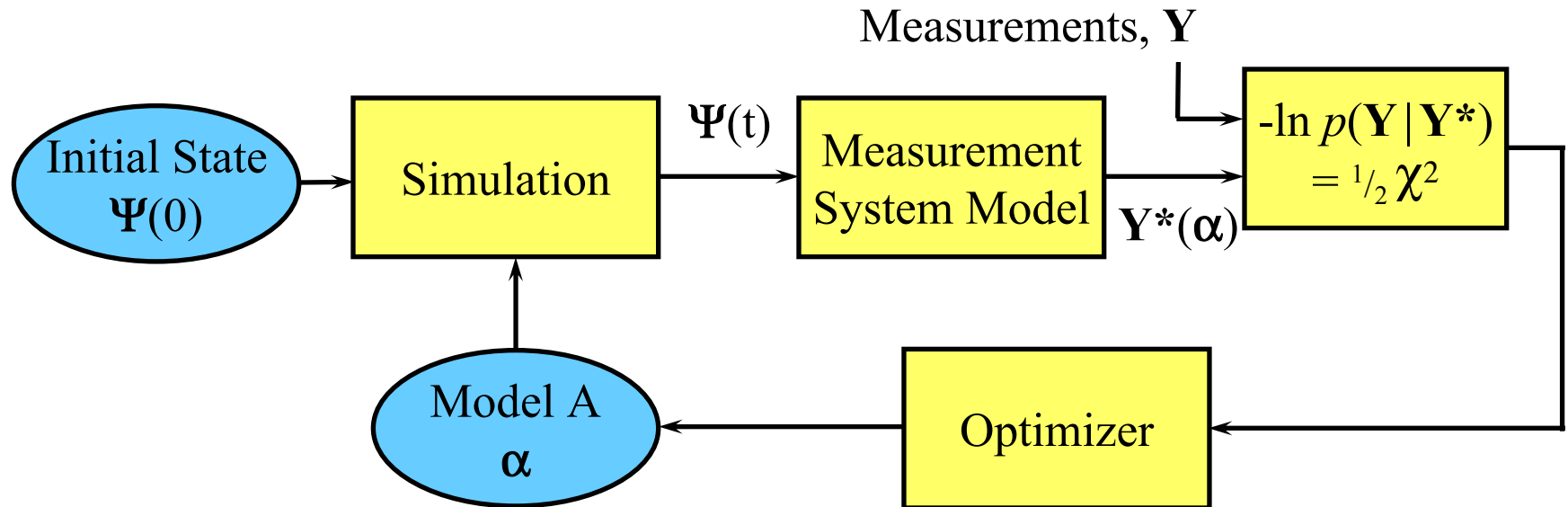
- Don't have measurements of the deformed cylinder yet, but suppose we do
- Quantitative comparison of simulation prediction with experimental data must take into account uncertainties in both

NESSUS/Abaqus



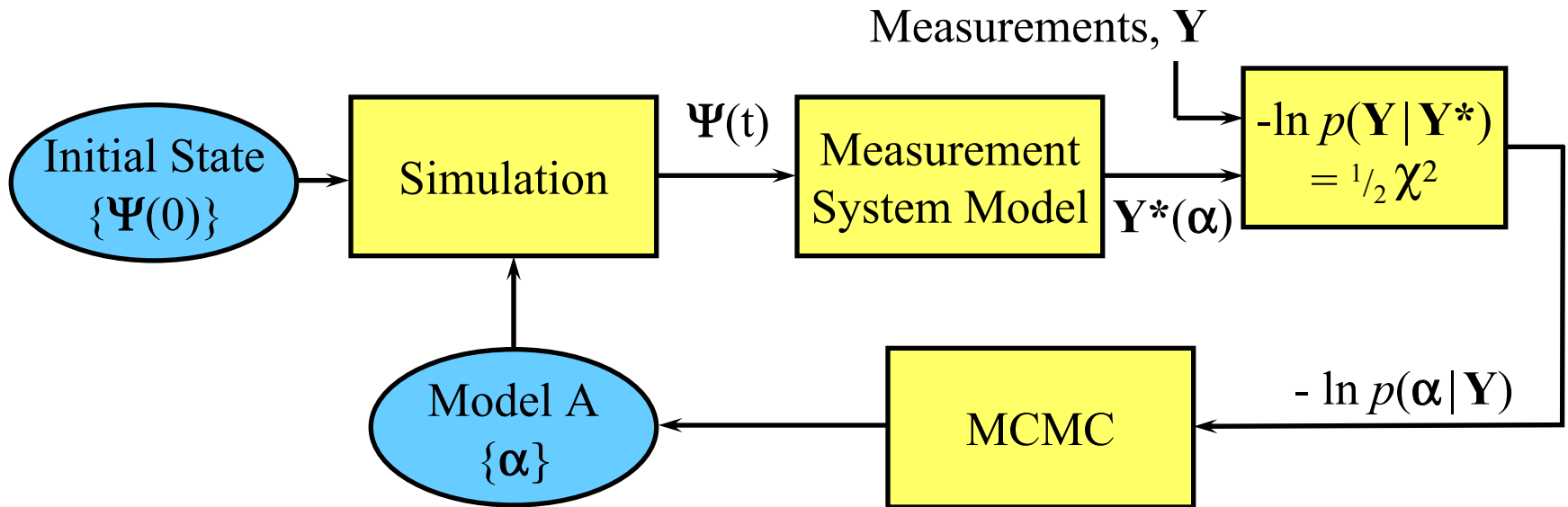
High-strength steel HSLA 100
246 m/s impact velocity

Parameter estimation - maximum likelihood



- Optimizer adjusts parameters (vector α) to minimize $-\ln p(Y | Y^*(\alpha))$
- Result is maximum likelihood estimate for α (also known as minimum-chi-squared solution)
- Optimization process is accelerated by using gradient-based algorithms along with adjoint differentiation to calculate gradients of forward model

Parameter uncertainties via MCMC



- Markov Chain Monte Carlo (MCMC) algorithm generates a random sequence of parameters that sample posterior probability of parameters for given data Y , $p(\alpha | Y)$, which yields plausible set of parameters $\{\alpha\}$.
- Must include uncertainty in initial state of system, $\{\Psi(0)\}$

Bayesian calibration strategy

- Hierarchy of experiments
 - ▶ basic - designed to isolate and characterize a basic physical phenomenon at single
 - ▶ partially integrated - involves more complex combination of phenomena, e.g., multiple materials, varying conditions, complex geometry, ...
 - ▶ fully integrated - attempt to approach application conditions
- Inference - use validation experiments to update info about model
 - ▶ capture info in terms of uncertainties
 - ▶ uncertainties indicate degree of confidence in prediction
 - ▶ attempt to develop model that is consistent with ALL available experiments
- Ultimate goal - Combine results from many (all) experiments
 - ▶ reduce uncertainties in model parameters
 - ▶ require consistency of models with all experiments

Bibliography

- ▶ “A framework for assessing confidence in simulation codes,” K. M. Hanson and F. M. Hemez, *Experimental Techniques* **25**, pp. 50-55 (2001); application of uncertainty quantification to simulation codes with Taylor test as example
- ▶ “A framework for assessing uncertainties in simulation predictions,” K. M. Hanson, *Physica D* **133**, pp. 179-188 (2000); an integrated approach to determining uncertainties in physics modules and their effect on predictions
- ▶ “Inversion based on complex simulations,” K. M. Hanson, *Maximum Entropy and Bayesian Methods*, pp. 121-135 (Kluwer Academic, 1998); describes adjoint differentiation and its usefulness in simulation physics
- ▶ “Uncertainty assessment for reconstructions based on deformable models,” K. M. Hanson et al., *Int. J. Imaging Syst. Technol.* **8**, pp. 506-512 (1997); use of MCMC to sample posterior

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